Calculating the dissociation chemistry and equation of state properties of materials

SAND2015-7275R

Tracking# (SAND, PR) _____

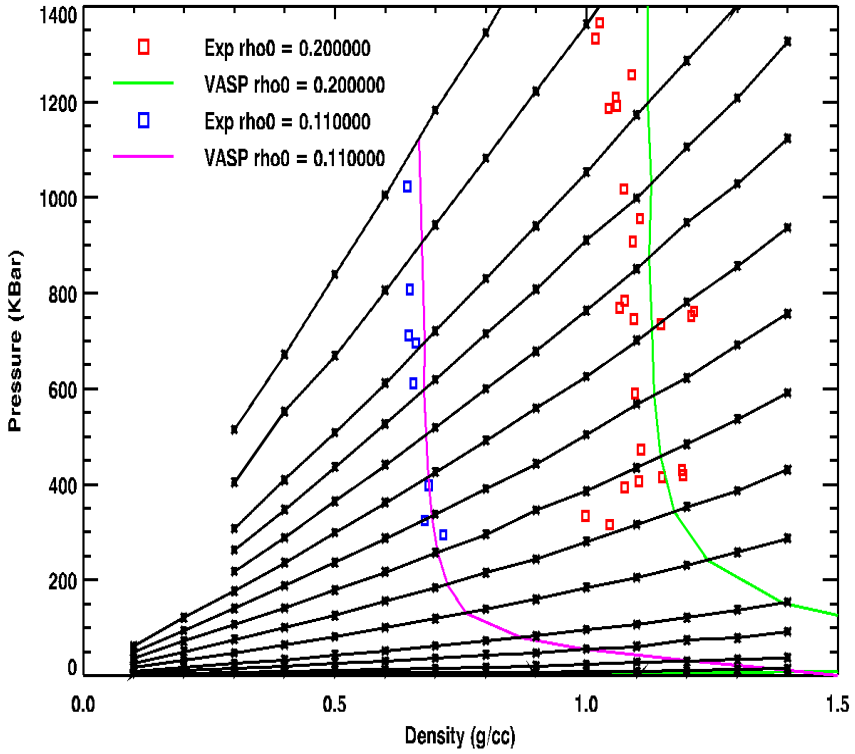
- Low density SiO_2 (aerogel) is used for a number of applications in many experiments
- Computational challenges
  - Low density requires a large simulation size and therefore, many cores
  - To build a general low density EOS requires many density/temperature pairs
  - Very long equilibration times. Each density/temperature pair needed 5 to 10 continuations
  - Critical points require more equilibration time than most other phases
- Proof of concept of new method for calculating the Hugoniot of porous materials

Principal Investigator: Kyle Cochrane

Platform and Campaign ID: Sequoia (CCC-127)

Usage: 1.5 Sequoia days

Aerogel EOS



This is a general aerogel EOS as calculated by VASP. Shown is a low density Hugoniot compared to experiment

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Calculating the dissociation chemistry and equation of state properties of materials (cont.)

Tracking# (SAND, PR) _____

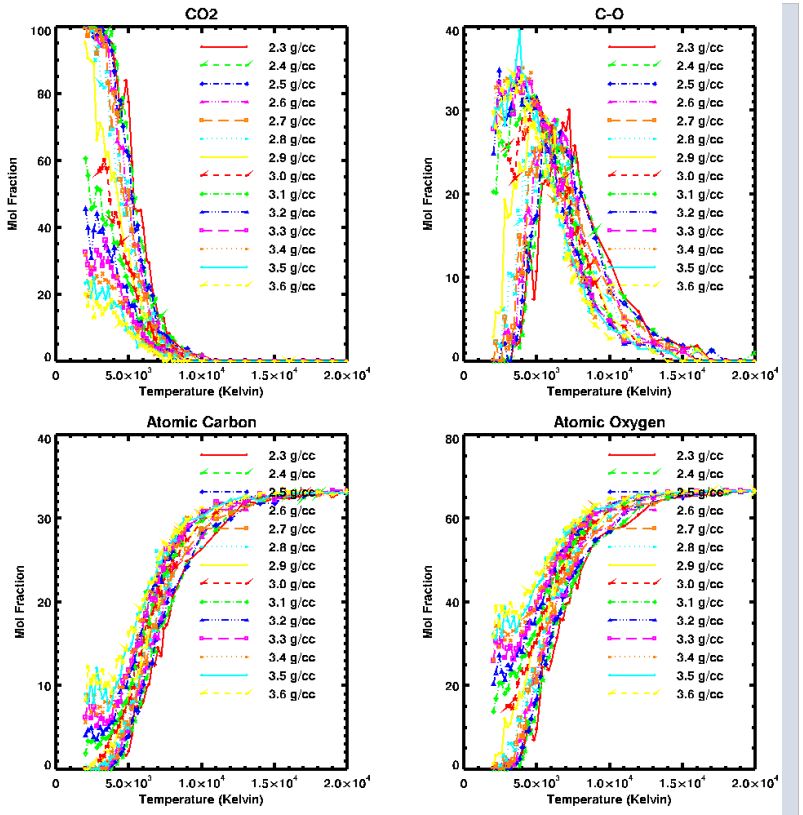
- We used VASP to calculate an EOS table in the compressed/shocked regime and track the chemical dissociation.
- Computational challenges
  - Require a large number of density/temperature pairs
  - To get accurate chemistry, need large number of atoms which requires large number of nodes
  - Very long equilibration times. Each density/temperature pair needed 5 to 10 continuations
- Sequoia's capacity made this project possible

Principal Investigator: Kyle Cochrane

Platform and Campaign ID: Sequoia (CCC-127)

Usage: 2.5 Sequoia days

Dominant Species of CO_2 during dissociation



These are the most populous species plotted as a function of temperature for constant density.

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Calculating the dissociation chemistry and equation of state properties of materials (cont.)

Tracking# (SAND, PR) _____

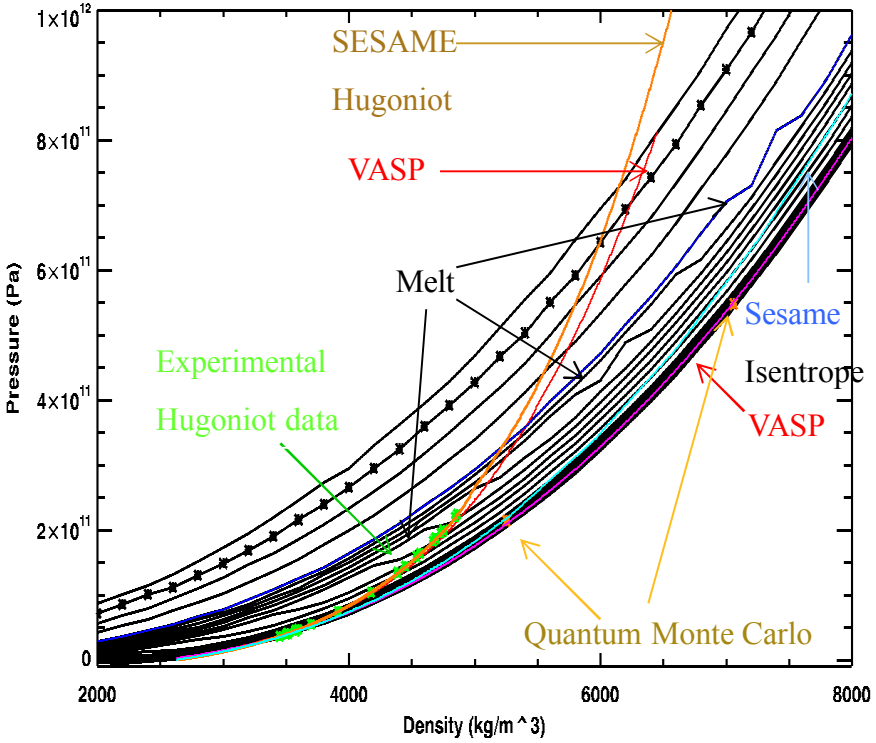
- Lithium Fluoride (LiF) is used as a window and an impedance standard for many shock experiments
- For this region of LiF, VASP runs fairly quickly
- Instead of calculating the individual parts (Hugoniot, isentrope, melt), it was easier to created a moderate range EOS and then calculate the parts from the EOS
- Agrees well with experiment. Shows flaws in current SESAME EOS table isentrope (cyan=SESAME, magenta=VASP)
- Shows melt in the same place that Riggs/Knudson experiment shows loss of signal and assumed due to melt

Principal Investigator: Kyle Cochrane

Platform and Campaign ID: Sequoia (CCC-127)

Usage: 1.0 Sequoia days

LiF EOS



This is a general LiF EOS as calculated by VASP. Shown is the table calculated values compared to SESAME and experiment.

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Calculating the dissociation chemistry and equation of state properties of materials(U)

Many experimental techniques are accurate enough to reveal glaring weaknesses in the material models used by physics codes to design them. This is requiring ever more stringent equation of state (EOS) development. Formerly, EOS models were built using limited gas gun shock data and a few general physics assumptions. With the ever increasing computer power available, we began using density functional theory (DFT) to approximate other EOS regimes such as the principal isentrope, critical point, and sometimes melt. With Sequoia, and only because of Sequoia's capacity, we are now calculating a limited range, general EOS table and then deriving the above EOS properties based on that table, often on a shorter time frame and more thoroughly than we used to compute just the EOS sections listed above.

The first project was to calculate a limited range EOS for CO_2 and specifically track the dissociated species present at each density and temperature. We would not see all of the possible species due to our small sample size and limited time, however, we should see the dominant species and general trends. This work was done to support a new, chemistry aware EOS model that is still under development at LANL.

The second project was done for two reasons. The first is LANL and SNL are developing a new amorphous SiO_2 EOS for use in hydrocodes. There is extensive principal Hugoniot and isentrope data, but very little lower density data. There is also no real estimate of the critical point so we found the approximate value of that as well. The second reason for lower density SiO_2 is to test a new method for calculating the Hugoniot of porous materials. Because aerogel (low density SiO_2) is used extensively in many shock experiments, there was a large data set to compare with. As can be seen in the figure, the new method appears to work well and is tracking the porous Hugoniot within the experimental error bars (not shown).

Finally, SNL is developing a new EOS for LiF because we were seeing discrepancies with the SESAME table. DFT has some issues calculating EOS values for LiF, so we will make some corrections, however, our first attempt appears to have very good results which confirm several experimentally seen properties, as seen on the previous slide.